JÜLICH
FORSCHUNGSZENTRUM

DOI-Vergabe für Großgeräte

im Journal of Large Scale Research Facilities JLSRF

23. Januar 2016 | Dr. Christoph Holzke, Dr. Claudia Frick, Dr. Bernhard Mittermaier

Das Anliegen

Woher kommen eigentlich die ganzen Daten die nun publiziert werden sollen?

- Von (verschiedenen) Autoren aus (verschiedenen) Forschungseinrichtungen

- Zum Teil aus Experimenten an großen Forschungsgeräten!
- BILDER von Groß(-groß)-geräten (Polarstern, MRT, HPC, Colider, Beamlines)

Das Großgerät wird im Abstract genannt …

„ First demonstrations of this setup at the coherence beamline of the ***PETRA III*** **storage ring** yield a highly divergent far-field diffraction pattern, from which the autocorrelation function of the near-field intensity distribution was obtained. “

DOI:10.1063/1.3698119

… oder im Acknowledgment

„And many thanks to the Alfred Wegener Institute for Polar and Marine Research (AWI) for providing the opportunity to join several research cruises across the Atlantic Ocean on ***RV Polarstern***, especially the expeditions ANT-XXIII/10, ANT-XXIV/1, ANT-XXIV/4, ANT-XXV/5 and ANT-XXVI/1.“

doi:10.5194/amt-5-2391-2012

… oder irgendwo

In the finite element context of Alya, the proposed gluing method consists in adding new elements, referred to as extension elements. These elements are assembled *almost* like normal finite elements (during the Assembly task) and do not require any particular treatment. Therefore the gluing method inherits the parallel performance in Alya. Figure 4 shows the speedup obtained on a Blue-Gene Q.

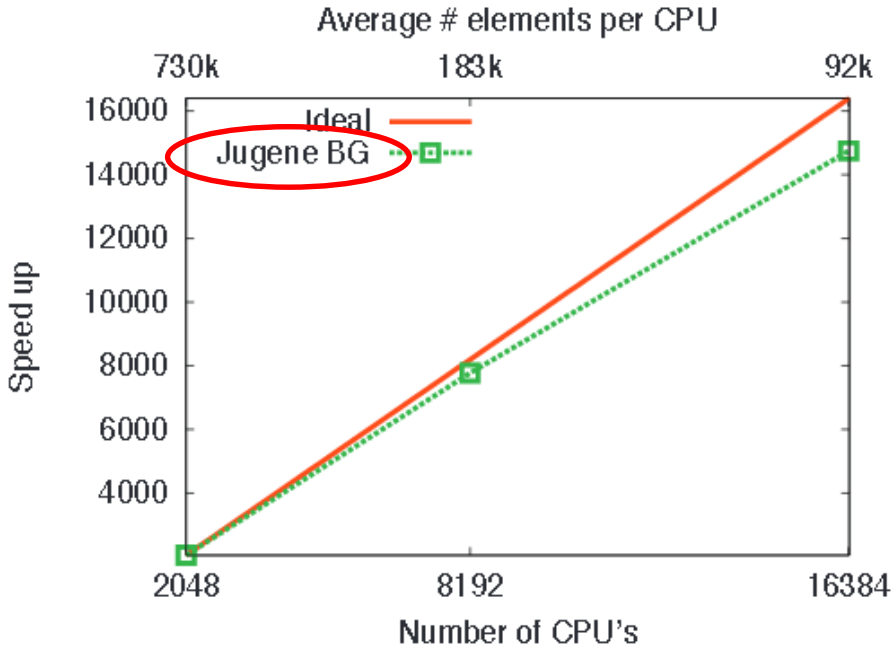


Figure 4 Alya speedup

DOI:10.1016/j.proeng.2013.08.013

Die Fragen

Großgeräte der Helmholtz-Gemeinschaft stehen den wiss. Communities für Experimente zur Verfügung

- Wie und von wem werden die Großgeräte genutzt?
- Welche Anteile haben Eigen- und Fremdnutzung?
- Erfüllt die HGF ihren Auftrag?
- Entwicklung von Experimenten

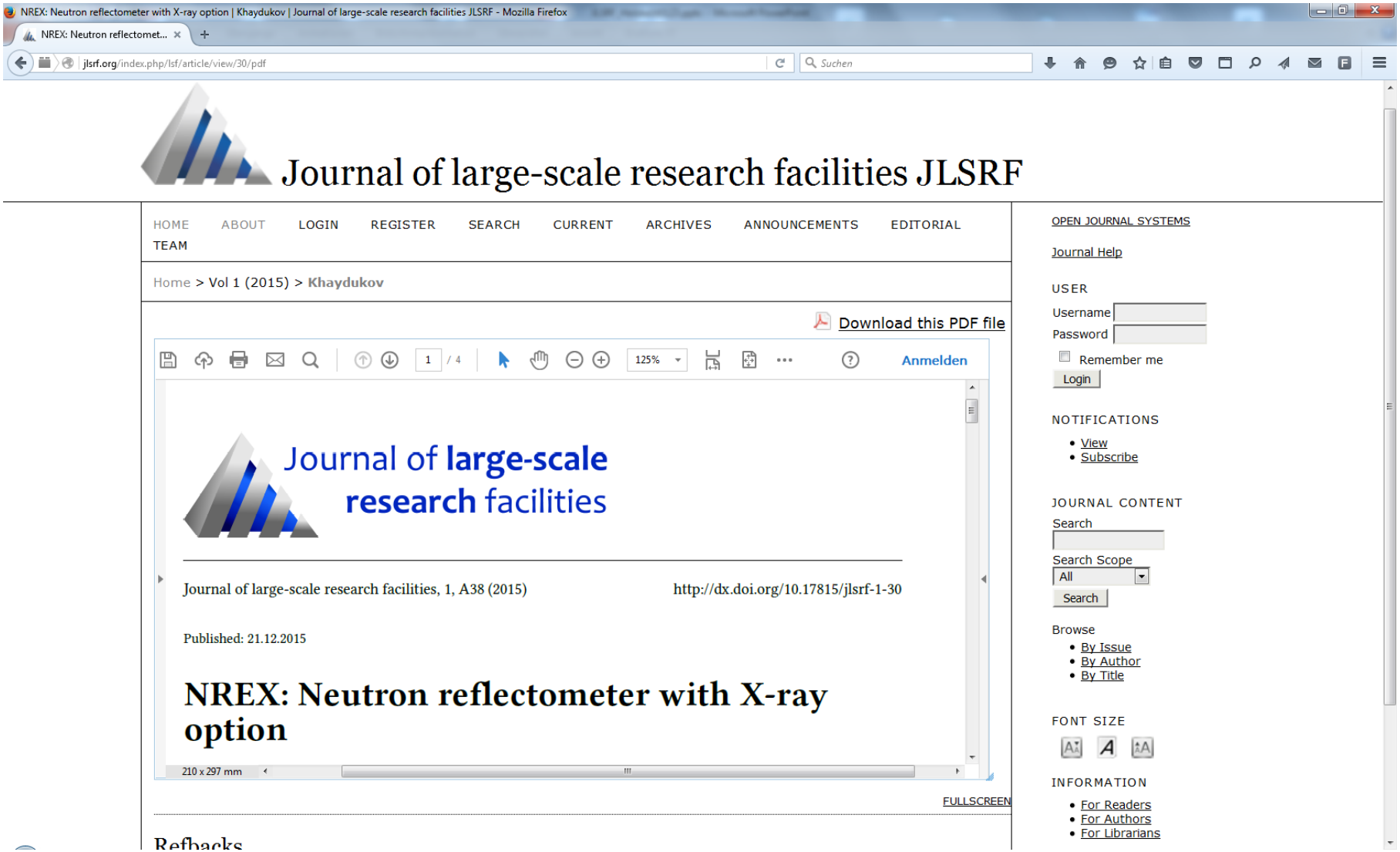
Das Anliegen

Zunächst auf Helmholtz-Ebene:

- HGF-Kernkompetenz Großgeräte verdeutlichen
- Sichtbarkeit der Geräte erhöhen
- Reputation für die Facilities
- Nachweis der lohnenden Investition

Die Idee: ***Großgeräte zitierbar machen***

Journal für den Nachweis „Großgeräte“



Beispiel

Journal of large-scale research facilities

Journal of large-scale research facilities, 1, A1 (2015) http://dx.doi.org/10.9999/example-doi

Published: 01.01.2015

BioDiff: The New Diffractometer for Crystals with Large Unit Cells

Heinz Maier-Leibnitz Zentrum

Instrument Scientists:
- A. Ostermann, Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany
- T. E. Schrader, Jülich Centre for Neutron Science (JCNS) at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany

Abstract: The BioDiff diffractometer is a new instrument built at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) in collaboration between the Forschungszentrum Jülich and the FRM II. It is optimised for studies of crystals with large unit cells and its main application lies in the structural analysis of protein crystals, more precisely in the determination of the position of the hydrogen atoms that are easily seen by neutron scattering but are normally not observed by X-ray crystallography. The BioDiff instrument is now in full user operation.

1 Instrument description

Since the human genome has been decoded and sequencing of the genome of other organisms has become a standard procedure the resulting information on the proteins encoded in these genomes can be used to express them in bacterial or yeast based expression systems and thereby study their interplay and function. One of the overall goals is a better understanding of the metabolism of a cell and thereby improving drugs and suppress side effects since they are tailored to attack only the part of the cell metabolism they are supposed to do so. In order to understand the function of a protein the knowledge of its three dimensional structure is a prerequisite. Often intermediate steps in the course of the catalytic process of a protein can be trapped and investigated with structure analysing techniques exhibiting atomic resolution, e.g. with X-ray or neutron diffraction. Here, the instrument BioDiff is able to perform neutron diffraction studies on protein crystals with comparatively large unit cells. The unique feature of BioDiff as compared to comparable instruments (e.g., LADI-III at ILL) is that the incident neutron wavelength can be adapted to the unit cell size of the sample crystal. Figure 1 shows a schematic view of the BioDiff instrument from the top and a corresponding picture when the biological shielding has been partly removed.
By Bragg reflection from a pyrolytic graphite crystal (002-reflection) neutrons are selected from the white spectrum of the neutron guide NL1 and pass through a first boron carbide adjustable slit and

1

: Schematic view of the BioDiff instrument (top) and a picture taken from a similar viewpoint e biological shielding removed (left).

selector. The latter acts as $\lambda/2$ filter. Together with the pyrolytic graphite crystal it forms chromator with a $\Delta\lambda/\lambda$ of $\sim 2.5\%$. Before entering the cylindrical drum of the image plate e beam is shaped by variable slits to fit to the sample size.
is equipped with two detectors. The cylindrical image plate detector (400*mm* in diameter and in height) is covering roughly half of the total 4π solid angle. It can be read out with three t resolutions of 125μm, 250μm and 500μm. As an alternative, one can lower the image plate r and swing in a neutron sensitive scintillator which is imaged onto a CCDchip.
CD-camera set-up serves as second detector but can also be used for the fast alignment of the crystal with respect to the neutron beam. The size of the scintillator is 197*mm* x 197*mm* and its e from the sample is 100*mm*. It can be moved around the sample to achieve 2Θ-values between 13°. Additionally, it can be displaced vertically by 100*mm*. Measuring at several positions, the lid angle coverage achievable with the CCD-detector amounts also to 2π.
tance tests for both detector types showed that the CCD-camera detector is comparable in sen- to the image plate detector, but covers only a smaller area (compare Figure 2). However, taking count the longer readout times of the image plate detector, the CCD-detector is an alternative of strongly scattering crystals. Here, the faster readout of the CCD-chip pays off even if the tector covers a smaller area.
the first 18 months of user operation 14 complete data sets of protein and DNA crystals were fully collected at BioDiff.

anned instrument development and upgrades

moment the crystal has to be taken off the instrument when one wants to tilt it in order to in- he completeness of the data set. This increases the risk to damage the crystal either mechanically ating it up when working under cryo-conditions. With a mini-kappa goniometer head as shown e 3 this can be avoided and an optimised tilt geometry can be chosen using special strategy e. This will help to collect the data more efficiently.
dity controlled gas stream can in some cases improve the crystal quality due to hydration and dation procedures with D_2O vapour (already tested at Proteros in Martinsried). It will also enable t variation techniques in low resolution crystallographic applications: e.g. lipids or detergents n be distinguished from the protein in membrane protein crystals. Better Lithium-ceramic flight ill help to reduce the background from air scattering of the primary beam. Illumination of the crystal with an optical fibre will allow to prepare and maintain intermediate states of photo- active proteins.

2

image plate

region of interest shown above recorded with CCD-detector

e image plate detector (upper part) compared to the same settings for

a variable tilt of the crystal while keeping it in the cold nitrogen gas e taken from Brockhauser, S. and Ravelli, R. B. G. and McCarthy, A. A. (2013).

3

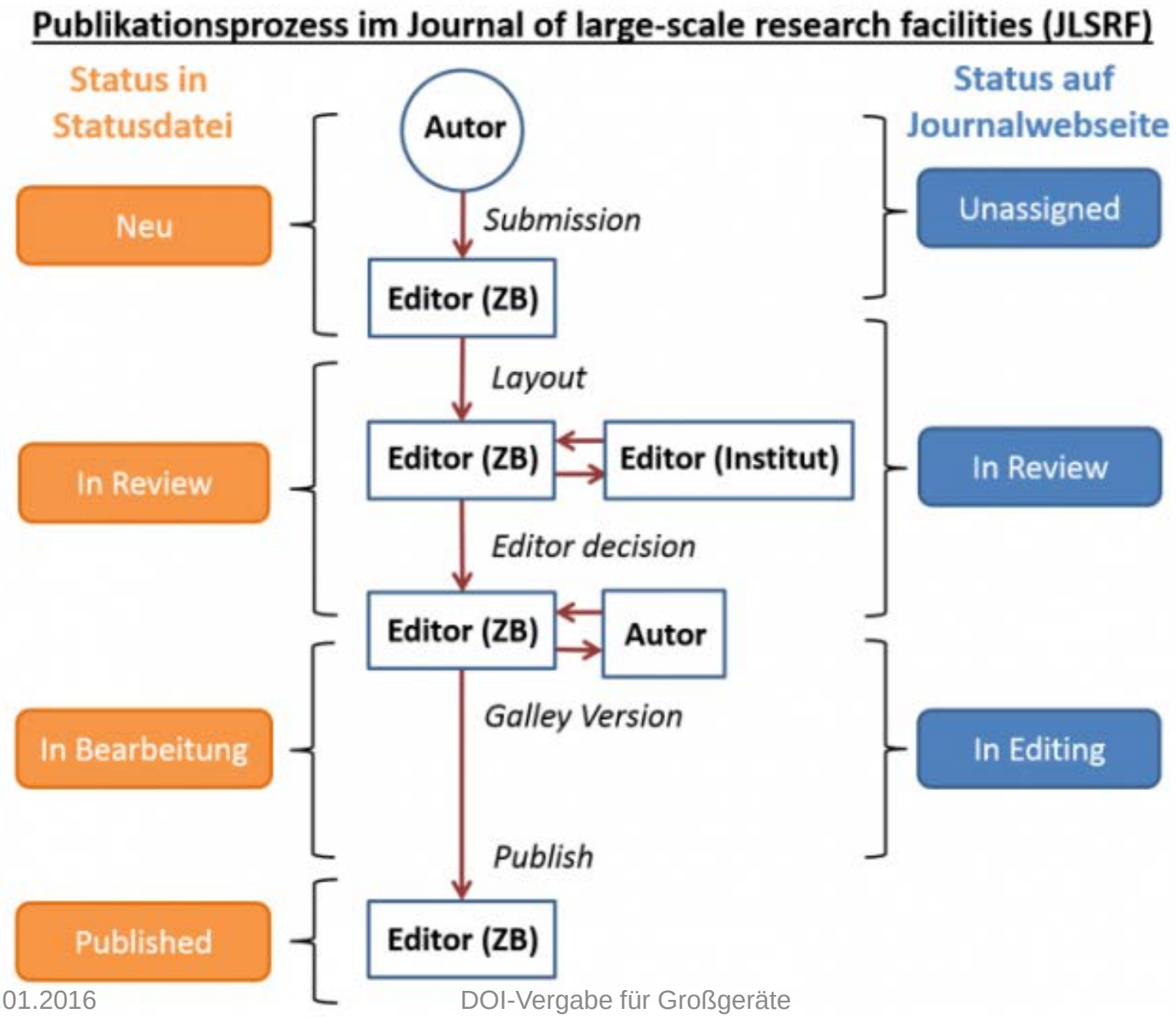
tend the existing wavelength range down to about 1.8Å utilising an nonochromator. This will close the gap to the thermal single crystal ng the application range of BioDiff to medium compound crystals.

eration where the protein crystal is typically mounted in a sealed e mother liquor BioDiff offers a standard Oxford Cryosystems 700+ ts in a nitrogen gas stream down to 90K. Additionally, a closed cycle temperatures down to 4K in vacuum for small compound crystals.

e neutron structure analysis of proteins, especially the determination tal fields of interest are:
tonation states of amino acids in the active center)
on shell of proteins
hydrogen bonds
monitor of structural stability/flexibility
roven to produce good quality crystallographic data sets and is now

, and McCarthy, A. A. (2013). The use of a mini-k goniometer head in y diraction experiments. *Acta Crystallographica Section D: Biological* 1251. http://dx.doi.org/10.1107/S0907444913003880

4



Wiki für unser Journal

Zeitschriften – QM-Wiki - Mozilla Firefox

Zeitschriften – QM-Wiki

wwwzb.fz-juelich.de/WIKIS/zb-qm/index.php?title=Zeitschriften

Suchen

QM hosted by JÜLICH FORSCHUNGSZENTRUM

Seite | Diskussion | Lesen | Quelltext anzeigen | Versionsgeschichte | Seite | Suchen

Übersicht

- QMH
- Verfahrensanweisungen
- Geschäftsgänge
- Standardarbeits-anweisungen
- Aufzeichnungen
- Formulardownload
- Archiv
- - Glossar

Navigation

- Hauptseite
- Gemeinschafts-Portal
- Aktuelle Ereignisse
- Letzte Änderungen
- Zufällige Seite
- Hilfe

Zeitschriften

Version 2.0	Verantwortlich
erstellt	C.frick 12:30, 16. Okt. 2015 (CEST)
geprüft	Ch. Esser 13:57, 22. Okt. 2015 (CEST)
freigegeben	B.mittermaier 14:35, 25. Okt. 2015 (CET)

Inhaltsverzeichnis [Verbergen]

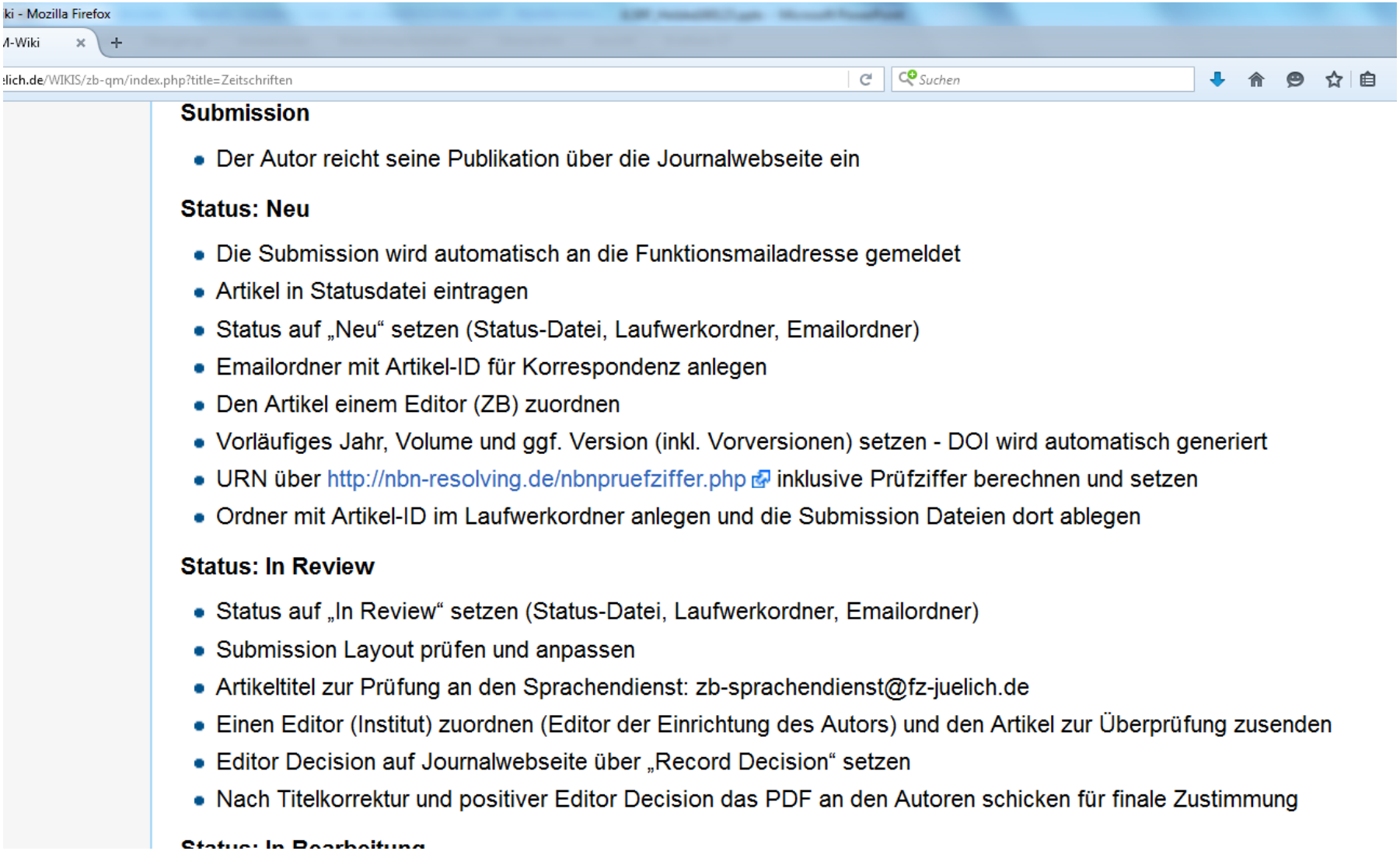
JLSRF Workflow

Zeitschriften

Journal of large-scale research facilities (JLSRF)

Der Status und der Stand der Zwischenschritte jeder Publikation werden fortlaufend in der Statusdatei festgehalten und aktualisiert. Die Statusdatei liegt auf einem Laufwerk zu dem alle Teammitglieder Zugang haben. Das selbe gilt für die Funktionsmailadresse.

Wiki für unser Journal



Submission

- Der Autor reicht seine Publikation über die Journalwebseite ein

Status: Neu

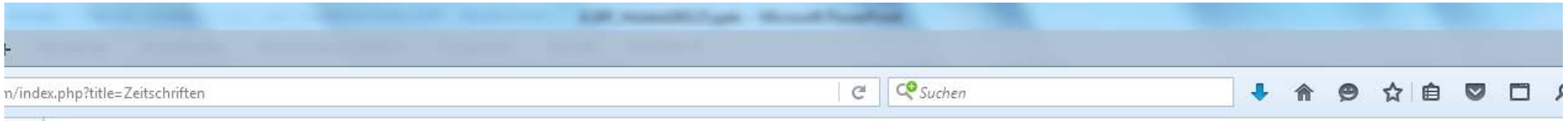
- Die Submission wird automatisch an die Funktionsmailadresse gemeldet
- Artikel in Statusdatei eintragen
- Status auf „Neu“ setzen (Status-Datei, Laufwerkordner, Emailordner)
- Emailordner mit Artikel-ID für Korrespondenz anlegen
- Den Artikel einem Editor (ZB) zuordnen
- Vorläufiges Jahr, Volume und ggf. Version (inkl. Vorversionen) setzen - DOI wird automatisch generiert
- URN über http://nbn-resolving.de/nbnpruefziffer.php inklusive Prüfziffer berechnen und setzen
- Ordner mit Artikel-ID im Laufwerkordner anlegen und die Submission Dateien dort ablegen

Status: In Review

- Status auf „In Review“ setzen (Status-Datei, Laufwerkordner, Emailordner)
- Submission Layout prüfen und anpassen
- Artikeltitel zur Prüfung an den Sprachendienst: zb-sprachendienst@fz-juelich.de
- Einen Editor (Institut) zuordnen (Editor der Einrichtung des Autors) und den Artikel zur Überprüfung zusenden
- Editor Decision auf Journalwebseite über „Record Decision“ setzen
- Nach Titelkorrektur und positiver Editor Decision das PDF an den Autoren schicken für finale Zustimmung

Status: In Bearbeitung

Wiki für unser Journal



Status: In Bearbeitung

- Status auf „In Bearbeitung“ setzen (Status-Datei, Laufwerkordner, Emailordner)
- Metadaten: Titel, Abstract, Referenzen (HTML für Links) und Autoren ggf. korrigieren oder ergänzen
- Fortlaufende Artikelnummer und Published Date setzen
- DOI und URN überprüfen und in die Metadaten eintragen
- Jahr, Volume, Artikelnummer, DOI und Published Date in das PDF eintragen
- Finales PDF auch als optimiertes PDF abspeichern
- Beide PDFs als „Galley Version“ auf die Journalwebseite hochladen, Benennung z.B. „Article A1“ und „Article A1 - small“
- Über „Scheduling“ das Volume auswählen, durch Klicken auf „Record“ wird der Artikel veröffentlicht
- Artikelnummer in „Table of contents“ auf der Journalwebseite eintragen

Status: Published

- Status auf „Published“ setzen (Status-Datei, Laufwerkordner, Emailordner)
- URN Erstanmeldung über DNB: https://admin.nbn-resolving.org/
- DOI Registrierung über CrossRef: https://doi.crossref.org (im XML „pages“ zu „article-number“ ändern)
- Pflichtabgabe bei der DNB: https://portal.dnb.de/delivery.htm (bei Stand/Version Artikelnummer und Version angeben, z.B. „A26, Version 0“)
- Elektronische Pflichtabgabe bei der ULB Bonn: http://epflicht.ulb.uni-bonn.de/publisher
- Finale Angaben in die Statusdatei eintragen
- Artikel zur Volumeliste hinzufügen
- Status auf „Fertig“ setzen (Status-Datei, Laufwerkordner, Emailordner)

Vielen Dank
für Ihre Aufmerksamkeit!

Dr. Christoph Holzke
Forschungszentrum Jülich
Zentralbibliothek
52425 Jülich
c.holzke@fz-juelich.de

Anhang

fraction, coming mainly from the power supplies, is still moved out of the rack by air. Engineered with fewer moving parts and built in redundancy, Blue Gene/Q has proven to be extreme reliable. Designed with a small footprint and low power requirements, Blue Gene/Q was ranked as the number-one most energy-efficient supercomputer in the world by the Green500 in Nov. 2011 (Green500, 2011).

References

Gauss Centre for Supercomputing. (2015). *Gauss Centre for Supercomputing e.V. (GCS).* Retrieved 05.05.2015, from http://www.gauss-centre.eu/

Green500. (2011). *The Green500 list.* Retrieved 05.05.2015, from http://www.green500.org/

Helmholtz Association. (2015). *Helmholtz-Gemeinschaft Deutscher Forschungszentren e.V. (HGF).* Retrieved 05.05.2015, from http://www.helmholtz.de/

Höchstleistungsrechenzentrum Stuttgart. (2015). *Höchstleistungsrechenzentrum Stuttgart (HLRS).* Retrieved 05.05.2015, from http://www.hlrs.de/

International Business Machines Corporation. (2013). The IBM Blue Gene/Q project. *IBM Journal of Research and Development*, *57*(1/2). http://dx.doi.org/10.1147/JRD.2012.2220487

http://dx.doi.org/10.1147/JRD.2012.2220487

International Business Machines Corporation. (2015). *IBM Blue Gene/Q information.* Retrieved 05.05.2015, from http://www.ibm.com/systems/technicalcomputing/solutions/bluegene/

Jülich-Aachen Research Alliance. (2015). *Jülich-Aachen Research Alliance – High-Performance Computing (JARA-HPC).* Retrieved 05.05.2015, from http://www.jara.org/en/research/jara-hpc/